

Nonequilibrium Temperature for Open Boson and Fermion Systems

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ABSTRACT

The effective theory of an open boson or fermion system is studied, which evolves out of equilibrium with a time-dependent Hamiltonian $\hat{H}(t)$. A measure of nonequilibrium temperature for the open system evolving from an equilibrium is proposed as the time-averaged energy expectation value $T(t) = T_i(\langle \hat{H}(t) \rangle_{\Psi} / \langle \hat{I}(t) \rangle_{\Psi})$, where $\hat{I}(t)$, the action operator, satisfies the quantum Liouville-von Neumann equation and determines the true density operator. It recovers the result for the adiabatic (quasi-equilibrium) and nonadiabatic (nonequilibrium) evolution from one static Hamiltonian to another and takes into account the particle production due to the intermediate processes.

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1 Introduction

A system becomes nonequilibrium (out of equilibrium) when its coupling constants change rapidly through the interaction with an environment. In inflationary scenarios, the inflation of the Universe would rapidly cool the inflaton and matter fields and this supercooling process would have happened far from equilibrium (see ref. [1]). Another phenomenon out of equilibrium is the recently introduced preheating mechanism, in which the parametric resonance of bosons and fermions coupled to the oscillating inflaton leads to catastrophic production of particles [2, 3, 4, 5, 6]. In quark-gluon plasma the second order phase transition out of equilibrium is expected to play an important role in quark-confinement [7, 8, 9]. Recently the nonequilibrium phase transitions have been actively studied to understand the dynamical process of domain growth and topological defects (see ref. [10]).

The quantum statistics, however, has not attracted much attention for these nonequilibrium systems though it is important in understanding the multi-particle phenomenon. Further a measure of temperature has not been assigned to such a nonequilibrium system because temperature is widely believed to make a physical sense only for an equilibrium system. But a quantum statistical theory has been proposed for nonequilibrium system based on the assumption that the microscopic world is correctly described by the Schrödinger equation and the quantum Liouville-von Neumann equation [11]. For the nonequilibrium system the frequently-used operator $\hat{\rho}_H(t) = e^{-\hat{H}(t)/kT}/Z_H$ cannot be used since it is *not* the true density operator. Instead the true density operator that satisfies the quantum Liouville-von Neumann is given by another operator $\hat{\rho}_I(t) = e^{-\hat{I}(t)/kT}/Z_I$, from which quantum statistics such as the Bose-Einstein or the Fermi-Dirac distribution is derived. Hence it may be suggested that the nonequilibrium temperature should be defined out of the Liouville-von Neumann operators $\hat{I}(t)$ and the dynamical energy operator $\hat{H}(t)$.

In this paper a quantitative measure of temperature is proposed for the nonequilibrium system. The analysis will be confined to the effective theory of an open boson or fermion system whose Hamiltonian $H(t)$ explicitly depends on time. The spatial homogeneity of the system will be assumed and the interaction among constituent particles will be neglected. The time-dependent nature of the system comes mainly from the interaction with an environment. Further, to simplify the analysis, we focus on the open boson or fermion oscillator with time-dependent frequency $\omega(t)$. The time-dependent boson oscillator has been extensively studied as an exactly solvable, nonstationary, quantum system [12, 13, 14]. Also an open fermion system has been studied as the nonequilibrium system [15]. For the time-dependent oscillator we derive the nonequilibrium temperature using the exact density operator $\hat{\rho}_I(t)$ and the Hamiltonian operator $\hat{H}(t)$ as giving the dynamical energy. Many solvable models are investigated, which evolve from one static Hamiltonian to another and have the limit of the adiabatic (quasi-equilibrium) or the nonadiabatic (nonequilibrium) evolution.

The organization of this paper is as follows. In Sec. II the relation between temperature and energy expectation value in the high temperature limit is discussed qualitatively and the temperature relation is derived approximately for the adiabatic and nonadiabatic evolution. In Sec. III, using the action operator and the exact density operator, the nonequilibrium temperature is defined by the ratio of the time-averaged energy expectation value to the expectation value of

the action operator. The nonequilibrium temperature is shown to be the quantum analog of the classical one from classical distribution function. In Sec. IV the nonequilibrium temperature is applied to several models of physical interest and extended to the time-dependent fermion system. In the nonadiabatic evolution from one static Hamiltonian to another, the final temperature is obtained in terms of the initial temperature, initial and final frequencies, and the particle production rate.

2 Adiabatic vs. Nonadiabatic Evolution

We start with an ensemble of boson oscillators with the frequency ω in a thermal equilibrium at temperature T . The thermal state of the system is described by the density operator $\hat{\rho}_H = e^{-\hat{H}/kT}/Z_H$ and has the energy expectation value

$$\langle \hat{H} \rangle_{\rho_H} = \frac{\hbar\omega}{2} \coth\left(\frac{\hbar\omega}{2kT}\right), \quad (1)$$

where \hbar is the Planck constant and k the Boltzmann constant. In the high temperature limit $kT \gg \hbar\omega$, the thermal energy expectation value has the limiting value

$$\langle \hat{H} \rangle_{\rho_H} = kT. \quad (2)$$

This may suggest that the temperature of the system should be derived from the energy expectation value at least in the high temperature limit.

We now evolve the system from one static Hamiltonian \hat{H}_i to another \hat{H}_f by adiabatically changing the frequency from ω_i to ω_f . If the system was in a thermal equilibrium, it would maintain quasi-equilibrium at each moment from the initial equilibrium to the final one. Both the initial and final states are assumed to have high temperatures. Then the ratio of the initial and final temperatures is given by the ratio of the corresponding energy expectation values:

$$\frac{T_f}{T_i} = \frac{\langle \hat{H}_f \rangle_{\rho_f}}{\langle \hat{H}_i \rangle_{\rho_i}}, \quad (3)$$

where ρ_i and ρ_f denote the initial and final density operators $\hat{\rho}_H$. If the density operator $\hat{\rho}_H$ does not change significantly, eq. (3) can be approximated by

$$\frac{T_f}{T_i} \simeq \frac{\langle \hat{H}_f \rangle_{\rho_i}}{\langle \hat{H}_i \rangle_{\rho_i}} = \frac{\omega_f}{\omega_i}. \quad (4)$$

The particle production due to the change of frequency (parameter) is negligible during the adiabatic evolution.

In the nonadiabatic evolution, the rapid change of frequency drives the system out of thermal equilibrium. Such a nonadiabatic process necessarily involves the particle production [16, 17, 18].

The creation and annihilation operators at the initial and final times are related with each other through the Bogoliubov transformation

$$\hat{a}(t_f) = \alpha \hat{a}(t_i) + \beta \hat{a}^\dagger(t_i), \quad \hat{a}^\dagger(t_f) = \alpha^* \hat{a}^\dagger(t_i) + \beta^* \hat{a}(t_i), \quad (5)$$

where the coefficients satisfy

$$\alpha^* \alpha - \beta^* \beta = 1. \quad (6)$$

It is interesting to compare the expectation values of the final and initial Hamiltonians with respect to the number states, $|n, t_i\rangle$, of initial time t_i , whose ratio is given by

$$\frac{\langle \hat{H}_f \rangle_{n_i}}{\langle \hat{H}_i \rangle_{n_i}} = \left(\frac{\omega_f}{\omega_i} \right) \times (1 + 2\beta^* \beta). \quad (7)$$

It therefore follows that

$$\frac{\langle \hat{H}_f \rangle_{\rho_i}}{\langle \hat{H}_i \rangle_{\rho_i}} = \left(\frac{\omega_f}{\omega_i} \right) \times (1 + 2\beta^* \beta). \quad (8)$$

The factor $\beta^* \beta$ is the number of particles created per unit volume and depends on the intermediate nonadiabatic process during the evolution. As will be shown later, eq. (8) is related to the temperature ratio. If a device measures the temperature of the system with time-averaged energy density, the final temperature would be given by

$$T_f = T_i \times \left[\frac{\omega_f}{\omega_i} (1 + 2\beta^* \beta) \right]. \quad (9)$$

3 Nonequilibrium Temperature

To define a quantitative measure of temperature that recovers eqs. (4) and (9) in the limiting cases, we study an open boson system described by a time-dependent oscillator

$$H(t) = \frac{p^2}{2} + \frac{\omega^2(t)}{2} q^2, \quad (10)$$

where the frequency $\omega(t)$ explicitly depends on time. The quantum states of the system are governed by the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi(q, t)}{\partial t} = \hat{H}(t) \Psi(q, t). \quad (11)$$

The statistical properties of the system are determined by the density operator that satisfies the quantum Liouville-von Neumann equation

$$i\hbar \frac{\partial \hat{\rho}(t)}{\partial t} + [\hat{\rho}(t), \hat{H}(t)] = 0. \quad (12)$$

The physical quantities which can be directly determined by eqs. (11) and (12) are $\langle \hat{H}(t) \rangle_{\Psi}$ and $\langle \hat{\rho}(t) \rangle_{\Psi}$, from which all other statistical variables such as the temperature and free energy will be derived. Here $|\Psi\rangle$ denotes any exact quantum state of eq. (11).

To find the exact quantum state of eq. (11), we use the idea of invariant operators first introduced by Lewis and Riesenfeld [19], who found a quadratic invariant of position and momentum. In refs. [20, 21, 11, 13], a pairs of linear invariant operators satisfying eq. (12) are introduced

$$\begin{aligned}\hat{a}^\dagger(t) &= -\frac{i}{\sqrt{\hbar}}[\varphi(t)\hat{p} - \dot{\varphi}(t)\hat{q}] \\ \hat{a}(t) &= \frac{i}{\sqrt{\hbar}}[\varphi^*(t)\hat{p} - \dot{\varphi}^*(t)\hat{q}],\end{aligned}\quad (13)$$

where φ is a complex solution to the classical equation

$$\ddot{\varphi}(t) + \omega^2(t)\varphi(t) = 0. \quad (14)$$

The Wronskian condition

$$\varphi(t)\dot{\varphi}^*(t) - \varphi^*(t)\dot{\varphi}(t) = i \quad (15)$$

guarantees the standard commutation relation

$$[\hat{a}(t), \hat{a}^\dagger(t)] = 1. \quad (16)$$

Hence the time-dependent operators $\hat{a}^\dagger(t)$ and $\hat{a}(t)$ play exactly the same role as the standard creation and annihilation operators. The Fock space of exact quantum states consists of the number states of $\hat{a}^\dagger(t)\hat{a}(t)$ [21]

$$\Psi_n(q, t) = \frac{1}{\sqrt{(2\hbar)^n n!}} \left(\frac{1}{2\pi\hbar\varphi^*\varphi} \right)^{1/4} \left(\frac{\varphi}{\sqrt{\varphi^*\varphi}} \right)^{(2n+1)/2} H_n \left(\frac{q}{\sqrt{2\hbar\varphi^*\varphi}} \right) \exp \left[\frac{i}{2\hbar} \frac{\dot{\varphi}^*}{\varphi} q^2 \right], \quad (17)$$

where H_n is the Hermite polynomial. The density operator satisfying eq. (12) is given by

$$\hat{\rho}_I(t) = \frac{1}{Z_I} e^{-\hat{I}(t)/kT_i}, \quad (18)$$

where

$$\hat{I}(t) = \hbar\omega_i \left[\hat{a}^\dagger(t)\hat{a}(t) + \frac{1}{2} \right]. \quad (19)$$

Here the free parameters T_i and ω_i will be fixed as the temperature and frequency, respectively, if the system starts from an initial equilibrium.

The action operator, $\hat{I}(t)$, gives an energy analog $\langle \hat{I}(t) \rangle_\Psi$ at each moment, where Ψ denotes the Fock state (17), whereas $\langle \hat{H}(t) \rangle_\Psi$ is the dynamical energy. We may write the expectation value of the density operator as

$$\langle \hat{\rho}_I(t) \rangle_\Psi = \frac{1}{Z_I} e^{-\langle \hat{I}(t) \rangle_\Psi / kT_i} = \frac{1}{Z_I} e^{-\langle \hat{H}(t) \rangle_\Psi / kT(t)},$$

where the time-dependent temperature is given by

$$T(t) \equiv T_i \times \left(\frac{\langle \hat{H}(t) \rangle_\Psi}{\langle \hat{I}(t) \rangle_\Psi} \right). \quad (20)$$

The process of taking the expectation value with respect to the Fock basis can be understood from the correspondence principle between quantum and classical theory. The classical density distribution is given by

$$\rho_I(t) = e^{-I(t)/kT_i} / Z_I, \quad (21)$$

where $I(t)$ is the classical action

$$I(t) = \omega_i \left[a^*(t)a(t) + \frac{1}{2} \right] \quad (22)$$

with the classical invariants [21]

$$\begin{aligned} a^*(t) &= -i[\varphi(t)p - \dot{\varphi}(t)q] \\ a(t) &= [\varphi^*(t)p - \dot{\varphi}^*(t)q]. \end{aligned} \quad (23)$$

The density distribution also can be written as

$$\rho_I(t) = \frac{1}{Z_I} \exp \left[-\frac{H(t)}{kT_c(t)} \right],$$

where

$$T_c(t) = T_i \times \left(\frac{H(t)}{I(t)} \right). \quad (24)$$

The temperature (20) is the quantum analog of the classical result (24), provided that the energy of $H(t)$ and $I(t)$ is evaluated appropriately in phase space.

A few comments are in order. First, the temperature relation (20) still holds even when $|\Psi\rangle$ is replaced by $\hat{\rho}_I(t)$. From the expectation values

$$\begin{aligned} \langle \hat{H}(t) \rangle_{\rho_I} &= \frac{\hbar}{2} \coth \left(\frac{\hbar\omega_i}{2kT_i} \right) [\dot{\varphi}^*(t)\dot{\varphi}(t) + \omega^2(t)\varphi^*(t)\varphi(t)], \\ \langle \hat{I}(t) \rangle_{\rho_I} &= \frac{\hbar\omega_i}{2} \coth \left(\frac{\hbar\omega_i}{2kT_i} \right), \end{aligned} \quad (25)$$

we find the temperature at any later time

$$\frac{T(t)}{T_i} = \frac{\langle \hat{H}(t) \rangle_{\rho_I}}{\langle \hat{I}(t) \rangle_{\rho_I}} = \frac{1}{\omega_i} [\dot{\varphi}^*(t)\dot{\varphi}(t) + \omega^2(t)\varphi^*(t)\varphi(t)]. \quad (26)$$

Second, if the time scale of oscillations determined by $\omega(t)$ is much smaller than the thermal relaxation time of measuring device, the time average should be taken over the period:

$$\bar{T} \equiv T_i \times \left(\frac{\overline{\langle \hat{H}(t) \rangle_{\Psi}}}{\overline{\langle \hat{I}(t) \rangle_{\Psi}}} \right). \quad (27)$$

Roughly speaking, the nonequilibrium temperature is determined by the time-averaged energy of the system at each moment.

4 Applications

We now consider the adiabatic or nonadiabatic evolution of boson oscillator from one static frequency ω_i to another ω_f . The solution to eq. (14) in general has the asymptotic form

$$\varphi_i(t) = \frac{e^{-i\omega_i t}}{\sqrt{2\omega_i}}, \quad (28)$$

$$\varphi_f(t) = \alpha \left(\frac{e^{-i\omega_f t}}{\sqrt{2\omega_f}} \right) + \beta \left(\frac{e^{+i\omega_f t}}{\sqrt{2\omega_f}} \right), \quad (29)$$

where α and β determine the Bogoliubov transformation (5) and satisfy the condition (6). The final state (17), into which eq. (29) is substituted, oscillates with the period π/ω_f . Then the temperature (27), obtained by taking the time average of eq. (26), is given by

$$\overline{T}_f = T_i \times \left[\frac{\omega_f}{\omega_i} (1 + 2\beta^* \beta) \right]. \quad (30)$$

The temperature (30) is the same as the temperature (9) of the nonadiabatic evolution, which was obtained qualitatively. It also reduces to the adiabatic result (4) when $|\beta| \ll 1$, that is, the particle production is negligible. So the temperature (27) recovers the nonadiabatic evolution from one static Hamiltonian in equilibrium to another.

We investigate the models with a parameter adjusting adiabaticity. The first model has the frequency which changes according to the modified Pöschl-Teller type [22]

$$\omega^2(t) = \omega_0^2 + \frac{\lambda(\lambda - 1)}{L^2 \cosh^2(t/\tau)}. \quad (31)$$

It has two asymptotic regions at $t \rightarrow \mp\infty$ with the same frequency ω_0 . The strength of interaction is determined by $\lambda(\lambda - 1)$ and the rate and duration by τ . The factor for pair production is given by

$$\beta^* \beta = \left(\frac{\sin \pi \lambda}{\sinh \pi \omega_0 \tau} \right)^2. \quad (32)$$

In the adiabatic limit of large τ ($\tau \gg 1$), the particle production is exponentially suppressed by $e^{-2\pi\omega_0\tau}$ and the result (3) is recovered. One prominent consequence is the temperature enhancement in the nonadiabatic limit of small τ ($\tau \ll 1$), which leads to $\beta^* \beta \gg 1$. Another model with an adiabatic parameter is given by the frequency

$$\omega^2(t) = \frac{1}{2}(\omega_i^2 + \omega_f^2) - \frac{1}{2}(\omega_i^2 - \omega_f^2) \tanh\left(\frac{t}{\tau}\right). \quad (33)$$

It also has two asymptotic regions at $t = \mp\infty$ with frequencies ω_i and ω_f , respectively. It is found [23]

$$\beta^* \beta = \frac{\sinh^2[\pi\tau(\omega_i - \omega_f)/2]}{\sinh(\pi\tau\omega_i) \sinh(\pi\tau\omega_f)}. \quad (34)$$

In the adiabatic limit of large τ , the particle production is again exponentially suppressed by $e^{-\pi\tau(\omega_i+\omega_f-|\omega_i-\omega_f|)}$. It is worth noting that in both models any nonadiabatic process with different τ leads to different final temperatures.

The next model is the preheating mechanism of light bosons or fermions coupled to an oscillating inflaton [2, 3, 4, 5, 6]. To simplify the analysis, we consider the model frequency of a scalar field mode

$$\omega^2(t) = \omega_0^2 + \theta(t)\omega_1^2 \cos \omega t, \quad (35)$$

where the parametric coupling to the inflaton turns on at $t = 0$. There are unstable narrow bands, in which the solution to eq. (14) grows exponentially due to the parametric resonance

$$\varphi_f \approx \frac{1}{\sqrt{2\omega}} \exp \left[-i\omega t + \frac{\omega_1^2}{2\omega} t \right]. \quad (36)$$

Then the temperature (27) is given by

$$\bar{T}_f \approx T_i \times \left[\frac{1}{2} \left\{ \frac{\omega}{\omega_0} + \frac{\omega_0}{\omega} + \frac{1}{\omega_0 \omega} \left(\frac{\omega_1^2}{2\omega} \right)^2 \right\} \right] e^{(\omega_1^2/\omega)t}. \quad (37)$$

The thermal energy of exponentially growing temperature comes from the decaying inflaton. The temperature (27) correctly describes the growing temperature in the preheating mechanism.

Finally, we extend the above analysis to the nonequilibrium system of time-dependent fermion oscillator. Pairs of fermions are also produced when the frequency changes in time [24, 18]. For an ensemble of fermion $(\hat{b}, \hat{b}^\dagger)$ and its antiparticle $(\hat{d}, \hat{d}^\dagger)$ with time-dependent parameters, pairs of linear invariant operators satisfying Eq. (12) are found in ref. [15]:

$$\hat{b}(t) = \alpha_b(t)\hat{b} + \beta_b(t)\hat{d}^\dagger, \quad \hat{b}^\dagger(t) = \alpha_b^*(t)\hat{b}^\dagger + \beta_b^*(t)\hat{d}, \quad (38)$$

$$\hat{d}(t) = \alpha_d(t)\hat{d} + \beta_d(t)\hat{b}^\dagger, \quad \hat{d}^\dagger(t) = \alpha_d^*(t)\hat{d}^\dagger + \beta_d^*(t)\hat{b}. \quad (39)$$

These operators satisfy the anticommutation relations

$$\{\hat{b}(t), \hat{b}^\dagger(t)\} = 1, \quad \{\hat{d}(t), \hat{d}^\dagger(t)\} = 1, \quad (40)$$

and all the other anticommutation relations vanish. The general result (20) or (27) holds with the new action operator

$$\hat{I}(t) = \hbar\omega_i[\hat{b}^\dagger(t)\hat{b}(t) - \hat{d}(t)\hat{d}^\dagger(t)]. \quad (41)$$

So, when the fermion system evolves from one static Hamiltonian \hat{H}_i with ω_i in an equilibrium to another \hat{H}_f with ω_f , we arrive at the final temperature

$$T_f = T_i \times \left[\frac{\omega_f}{\omega_i} (1 + \beta_b^*\beta_b + \beta_d^*\beta_d) \right]. \quad (42)$$

The above temperature, which is valid for the adiabatic ($\beta = 0$) and nonadiabatic ($\beta \neq 0$) evolution, is the fermion analog of the boson result (30). The coefficient relations due to the anticommutation relations

$$\alpha_i^*\alpha_j + \beta_i^*\beta_j = \delta_{ij}, \quad i, j = a, b, \quad (43)$$

limit the fermion production due to the Pauli-blocking.

5 Conclusion and Discussion

We have studied the nonequilibrium evolution of a time-dependent boson or fermion system and proposed the nonequilibrium temperature through eq. (20) or (27). The quantum statistics is defined quantitatively and rigorously for the nonequilibrium system under the assumption of the Schrödinger equation (quantum law) and the quantum Liouville-von Neumann equation. For the time-dependent boson or fermion oscillator these two equations can be solved simultaneously in terms of quantum invariant operators, which in turn can be found in terms of classical solutions of motion. The true density operator is constructed from a particular quantum invariant $\hat{I}(t)$, called the action operator. Using the well-known fact that in the high temperature limit the energy expectation value of a thermal ensemble of boson or fermion oscillator is proportional to the temperature, we define the nonequilibrium temperature (20) or (27) from the dynamical energy of the Hamiltonian operator $\hat{H}(t)$ and that of the action operator $\hat{I}(t)$ of the true density operator. It recovers the temperature (9) for the nonadiabatic evolution from one static Hamiltonian to another, not necessarily in equilibrium. The nonequilibrium temperature is applied to many physical models in Sec. VI.

Finally we discuss whether the nonequilibrium temperature (20) or (27) can be applied to a system whose final static Hamiltonian has a lower temperature. In the lower temperature limit the vacuum energy dominates over thermal energy and leads to the expectation value

$$\langle \hat{H} \rangle_{\hat{\rho}_H} = \frac{\hbar\omega}{2}. \quad (44)$$

Therefore it seems that the qualitative derivation of temperature in Sec. II fails in this model. However, the direct analysis below shows that the temperature (20) or (27) may still be applied to this model. As a temperature lowering model, we consider a second order phase transition, which is described by the sign changing frequency

$$\omega^2(t) = \theta(-t)\omega_i^2 - \theta(t)\omega_f^2. \quad (45)$$

Here θ is the step function which takes $\theta(t) = 1$ when $t > 0$ and $\theta(t) = 0$ when $t < 0$. The solution to eq. (14) is given by

$$\begin{aligned} \varphi_i(t) &= \frac{e^{-i\omega_i t}}{\sqrt{2\omega_i}}, \\ \varphi_f(t) &= \frac{1}{\sqrt{2\omega_f}} \left[\cosh(\omega_f t) - i \frac{\omega_i}{\omega_f} \sinh(\omega_f t) \right] \end{aligned}$$

The expectation value $\langle \hat{H}(t) \rangle_{\Psi}$ with respect to any number state (17) vanishes because the kinetic and potential energies contribute equally with opposite signs [11]. The final temperature T_f approaches zero when the instantaneous quench process continues for a sufficiently long time. In a finite quench the final temperature needs not to be exactly zero. This implies that the temperature proposed in this paper may have a wide range of validity including the lower temperature region.

Not considered in this paper is the process of the nonequilibrium system evolving toward the final equilibrium state with the true density operator $\hat{\rho}_H = e^{-\hat{H}_f/kT_f}/Z_H$. The effective theory of

time-dependent boson or fermion oscillator cannot describe this process properly since the final states oscillate rapidly. To get the non-oscillating final Fock states, the final solution to eq. (14) should have the form (28), which in turn leads to the initial solution of the form (29). This implies that our effective theory of the open system cannot describe completely the nonequilibrium process from one equilibrium to another. Even with the more elaborated model that describes correctly the evolution from one equilibrium to another, the particle production due to the nonadiabatic process leads to the chemical potential. These points together with statistical relations will be addressed in a future publication.

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